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Catalysis Today 113 (2006) 220–225
CATALYSIS TODAY
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Magnetic structure of fcc Fe films on Co(1 1 1)

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Available online 31 January 2006

Abstract

The collinear magnetic structure of n ($n = 1, \ldots, 6$) monolayers (ML) of Fe films deposited on Co(1 1 1) substrate is investigated by ab initio density functional theory within a generalized gradient approximation. We have found that the ferromagnetic ground state exists only for one Fe monolayer. For higher thickness, a sequence of antiferromagnetic coupling with low magnetic moments in the inner layers of films is identified as ground state.

Keywords: Magnetic structure; fcc Fe films; Co substrate

1. Introduction

The strong correlation between structural and magnetic properties of face centred cubic (fcc) Fe films deposited on copper substrate with different crystallographic orientations and on cobalt with (1 0 0) direction, have been the subject of extensive researches. Several experimental techniques such X-ray magnetic circular dichroism (XMCD) [1], magneto-optic Kerr effect (MOKE) [2] and photoemission [3] have been extensively used for the exploration of the magnetism and structural details of fcc Fe films, in particular their dependence on the Fe film thickness. On Cu(1 0 0), Fe films assume a ferromagnetic (FM) face centred tetragonal (fct) structure for thickness below 4 monolayers (ML) (region I) and an antiferromagnetic (AFM) fcc structure at thickness between 5 and 11 ML (region II). For these thicknesses, the stabilization of this structure is due to the expansion of interlayer distances between ferromagnetically coupled layers and a contraction of distances for antiferromagnetically coupled layers [4]. Fe films thicker than 11 ML transform in FM body centred cubic (bcc) phase (region III) [1,2,5]. Comparing reflexion high-energy diffraction (RHEED) oscillations results and magnetic measurement by MOKE technique, Escrocia-Aparicio et al. [2] have observed the same structural and magnetic behaviors in Fe/Co(1 0 0) than those of Fe/Cu(1 0 0) with small difference in magnetic moments due to substrate polarization. By XMCD technique, Schmitz et al. [5] have found that the Fe spin moment is 3 μ_B on Co(1 0 0) and 2.8 μ_B on Cu(1 0 0) in region I. In region II, it decreases to 1.1 and 0.8 μ_B for Fe/Co(1 0 0) and Fe/Cu(1 0 0), respectively. For a Fe thickness larger than 10 monolayers, the magnetic moment in the Fe coverage increases again.

From theoretical studies [4,6], Asada and Blügel [6] have investigated the collinear magnetism of n ($n = 1, \ldots, 6$) monolayers of Fe films deposited on Cu(1 0 0) using full-potential linearized augmented plane-wave (FLAPW) method. They have found that FM order is the ground state up to 3 ML, whereas above this thickness, Fe films present a bilayer AFM coupling for an even number of monolayers, and a sequence of several spin states for an odd number. Therefore, the magnetic transition from the FM to the AFM states occurs for $n = 3$ ML, whereas the experimental result [5] predicts a magnetic transition for $n = 4$ ML. This discrepancy can be explained by the perfect interface considered in theoretical studies. Indeed, in experimental investigations, such perfect interfaces do not exist, because the Fe films growth is accompanied by the apparition of roughness, interdiffusion effects and complex reconstructions at the interface [7,8] which have a strong influence on the magnetism and structure of Fe films [9–11]. Those effects lead to the formation of spin spiral density wave [12–20].

In order to provide additional information about electronic effects of the substrate nature on the magnetic phases of fcc Fe

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doi:10.1016/j.cattod.2005.11.086

films, the magnetic structure of Fe/Co(1 0 0) system has also been studied using ab initio calculations. Using tight binding linear muffin-tin orbital with atomic sphere approximation (TB-LMTO-ASA) method within local spin density approximation (LSDA), Mokrani et al. [21] have found that the Fe films are ferromagnetic only for one and two monolayers. However, because the LSDA does not give the correct Fe magnetic ground state [22], Spišák and Hafner [23] have used ab initio local spin density technique including generalized gradient corrections (GGC) to investigate Fe/Co(1 0 0) magnetism. Up to three monolayers, they have found similar results than those of Mokrani et al. [21] with however a considerable difference in the magnetic moments and energy differences. In addition, they have found that above 3 ML, Fe films produce a bilayer AFM ground state for an even number of Fe layers, while for an odd number, several spin structures coexist. The failure to predict ferromagnetism in Fe films with three and four monolayers as observed experimentally has been attributed to the influence of the epitaxial constraint of Co/Cu(1 0 0) on the magnetism of Fe films since the fcc structure of Co is stabilized by epitaxial growth on Cu(1 0 0) [1]. Another factor that could affect the magnetism of fcc Fe films is the intermixing Fe–Co at the interface since Co and Fe show a large mutual solubility.

Today, interest is focused on growth and magnetism of fcc Fe films on Cu(1 1 1) surface. Experimentally, it was shown that, by using thermal deposition (TD), Fe films on Cu(1 1 1) undergo a transition from fcc low-spin (LS) to bcc high-spin (HS) ferromagnetic states for three monolayers [24], while by pulse laser deposition (PLD), an isomorphic fcc Fe is stabilized up to six monolayers [25,26]. The oscillations of total magnetic moment as a function of film thickness have been determined by MOKE technique [25], where it was observed that magnetic phase transformation from HS-FM to LS-FM order occurs at a thickness of about three monolayers. The article of Shen et al. [27] gives a description of the structure, morphology and magnetism of ultrathin Fe films epitaxially grown on Cu(1 1 1) surface. However, very few calculations have been devoted to magnetic and structural properties of those systems. In their study of magnetism of transition metals on Cu(1 1 1) and Ag(1 1 1) substrates, Krüger et al. [28] have found ferromagnetic order as ground state for 1 ML of Fe/Cu(1 1 1). In addition, Krüger [29] has studied the collinear magnetism of Fe films deposited on Cu(1 1 1) for thickness up to six monolayers using TB-LMTO-ASA based on both GGA and LSDA approximations. This author found that for the GGA approach, the ground state is ferromagnetic up to 3 ML while this FM coupling is stable only for 2 ML for the LSDA approximation. Comparing magnetic behavior of Fe films as function of their thickness with experimental data, he found similar oscillatory behavior. He attributed this spin transition to a competition between surface/interface effects and preferentially ferromagnetic coupling between adjacent monolayers on one hand and bulk like spin-density wave correlations on the other hand. In their recent study, Spišák and Hafner [30] have proved that as for Fe/Cu(1 0 0), the magnetism of fcc Fe films on Cu(1 1 1) is strongly coupled to structure distortions.

In the literature, several attempts have been made to study the magnetic behavior of Fe films deposited on Cu(1 0 0), Co(1 0 0) and Cu(1 1 1) substrates, but, until now, there are no theoretical nor experimental investigations on the magnetic structure of Fe/Co(1 1 1). As it is well known, the magnetic properties of ultrathin films depend on the details of atomic structure, it is therefore, worthwhile to determine the magnetic behavior of fcc Fe films on Co(1 1 1) and compare it with [1 0 0] direction in order to understand the effect of symmetry and coordinations number change. This aspect constitute the first aim of our study. The second motivation of this work is to compare the general trends and to highlight both common and distinct properties obtained for Fe/Co(1 1 1) with those of Fe/Cu(1 1 1) system.

The rest of this paper is organized as follows: After a brief account in Section 2 of the theoretical model used for calculations in the framework of the TB-LMTO-ASA method, the results of the magnetic map of Fe/Co(1 1 1) are presented and discussed in Section 3. The main conclusions of the study are summarized in the last section.

2. A brief outline of the method

The collinear magnetic calculations of Fe films on Co(1 1 1) are performed using a scalar-relativistic version of the k-space tight binding linear muffin-tin orbitals with atomic sphere approximation (TB-LMTO-ASA) method [31,32]. Since the LSDA approach cannot give the correct ground state of ferromagnetic bcc Fe [4,22,33], we have used the generalized gradient approximation with Langreth-Mehl-Hu functional (GGA-LMH) [34]. Several studies have been done for magnetic properties of bulk fcc Fe [35,36] and they have shown that its magnetic ground state is AFM with an equilibrium lattice parameter of 6.56 a.u. and magnetic moment of 1.0 μ_B. This lattice parameter is used in our study. The choice of GGA-LMH [34] approximation is also a result of our calculations of equilibrium lattice parameter of fcc Co in bulk. As shown in Table 1, the lattice constant of fcc Co (a = 6.63 a.u.) and magnetic moment (μ = 1.63 μ_B) obtained from the GGA-LMH are in good agreement with experimental parameter (a = 6.68 a.u., μ = 1.61 μ_B) [37] and with previous calculation Spišák and Hafner [23] (a = 6.64 a.u). In order to investigate magnetic properties of Fe films, we have used the super-cell technique. Since the experimental studies [41]

Table 1
Lattice parameter (in a.u.) of Co bulk calculated with LSDA of Vosko-Wilk-Nusar (VWN) [38] and von Barth-Hedin (v.BH) [39] functional and with GGA of Perdew-Wang (PW91) [40] and Lagnreth-Mehl-Hu(LMH)[34] functional compared to the experimental one [37]

Exchange-correlation functional	LSDA		GGA		Exp.
	vBH	VWN	LMH	PW91	
Lattice parameter Co(fcc) (a.u.)	6.55	6.56	6.63	6.80	6.68
Magnetic moment (μ_B/atom)	1.57	1.62	1.63	1.69	1.61